

# **SUPPLEMENTAL MATERIAL FOR**

## **Endocrine Disruptors and Asthma-Associated Chemicals in Consumer Products**

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Table S1. Chemical class summaries, including uses, potential health effects, and compounds analyzed.

| Chemical Class | Use(s) in Products <sup>a</sup>   | Potential Health Concerns <sup>b</sup>   | Chemicals   |
|----------------|---|--|---|
| parabens       | preservative; anti-microbial agent  | endocrine disruption (Kang et al. 2002)  | methyl paraben<br>ethyl paraben<br>butyl paraben  |
| phthalates     | plastic additives; solvents in cosmetics and perfumes; inert ingredient in pesticides | endocrine disruption (Hannas et al. 2011; Hauser et al. 2006; Heindel et al. 1989; Howdeshell et al. 2008; Meeker et al. 2009; Mendiola et al. 2011; Swan et al. 2005).<br>asthma associated (Bornehag et al. 2004; Bornehag and Nanberg 2010) | bis(2-ethylhexyl) adipate<br>bis(2-ethylhexyl) phthalate<br>benzylbutyl phthalate<br><i>di-amyl phthalate</i><br>di-cyclohexyl phthalate<br>di-isobutyl phthalate<br>di-isononyl phthalate<br>di-n-butylphthalate<br>di-n-hexyl phthalate<br>di-n-octyl phthalate<br>di-n-propyl phthalate<br>diethyl phthalate |
| bisphenol A    | production of polycarbonate plastic and epoxy resins                                  | endocrine disruption (FAO/WHO 2010; NTP-CERHR 2008)  | bisphenol A   |
| antimicrobials | anti-microbial agent  | endocrine disruption (Chen et al. 2008; Orton et al. 2011; Stoker et al. 2010)   | <i>1,4-dichlorobenzene</i><br><i>o-phenylphenol</i><br>triclosan<br>triclocarban  |
| ethanolamines  | solvent in cleaners; emulsifier in creams and lotions                                 | asthma associated (Kamijo et al. 2009; Makela et al. 2011; Piipari et al. 1998; Savonius et al. 1994)  | monoethanolamine<br>diethanolamine  |
| alkylphenols   | surfactant; disinfectant; inert ingredient in pesticides                              | endocrine disruption (Jie et al. 2010)   | 4-t-octylphenol<br>octylphenol monoethoxylate<br>octylphenol diethoxylate<br>4-t-nonylphenol<br>nonylphenol monoethoxylate<br>nonylphenol diethoxylate  |

| Chemical Class | Use(s) in Products <sup>a</sup>    | Potential Health Concerns <sup>b</sup>   | Chemicals  |
|----------------|------------------------------------|--|--|
| fragrances     | scent; masking agent               | endocrine disruption (Bitsch et al. 2002; Schreurs et al. 2005; Seinen et al. 1999; van der Burg et al. 2008)<br>asthma associated (Kumar et al. 1995) | <u>natural<sup>c</sup></u><br>benzyl acetate<br>eugenol<br>hexyl cinnemal<br>limonene<br>linalool<br>methyl eugenol<br>methyl salicylate<br>pinene<br>terpineol  |
|                |                                    |  | <u>synthetic</u><br>AHTN<br>bucinal<br>diphenyl ether<br>DPMI<br>HHCB<br>isobornyl acetate<br>methyl ionone<br>musk ketone<br>musk xylene<br>phenethyl alcohol   |
| glycol ethers  | solvent                            | asthma associated (Choi et al. 2010)   | 2-isopropoxyethanol (R2)<br>2-propoxyethanol (R2)<br>2-butoxyethanol<br>2-phenoxyethanol (R2)<br>2-benzyloxyethanol (R2)<br>2,2-methoxyethoxyethanol<br>2,2-ethoxyethoxyethanol (R2)<br>2,2-butoxyethoxyethanol (R2) |
| perfluorinated | stain resistance                   | endocrine disruption (White et al. 2011)   | 8:2 FTOH   |
| cyclosiloxanes | enhance conditioning and spreading | endocrine disruption (Quinn et al. 2007)<br>carcinogenicity (Wang et al. 2009)   | octamethylcyclotetrasiloxane (D4) (R2)<br>decamethylcyclopentasiloxane (D5) (R2)<br>dodecamethylcyclohexylsiloxane (D6) (R2)   |

| Chemical Class | Use(s) in Products <sup>a</sup>                   | Potential Health Concerns <sup>b</sup>      | Chemicals  |
|----------------|---|---|--|
| UV filters     | skin protection; product stability and durability | endocrine disruption (Schlumpf et al. 2004) | <i>3,4-methylbenzylidene camphor</i> (R2)<br>benzophenone (R2)<br>benzophenone-1 (R2)<br><i>benzophenone-2</i> (R2)<br>benzophenone-3 (R2)<br>oxtinolate (R2)<br><i>octadimethyl PABA</i> (R2) |

<sup>a</sup> General use categories obtained from the NLM Hazardous Substance Data Bank and/or scientific literature

<sup>b</sup> Health effects have not necessarily been reported for all chemicals within the chemical class. Among the EDCs in this study, phthalates are the only chemical group for which there is supporting evidence of health effects from human studies. All asthma-associations are derived from human studies.

<sup>c</sup> Natural fragrances are readily available from plant materials, but can also be synthesized. Stereoisomer composition will differ for chemically synthesized materials. Our analysis did not determine whether these were synthesized or derived from plant materials.

R2 indicates chemicals added during the second round of sampling

Italicized chemicals were not detected in any product

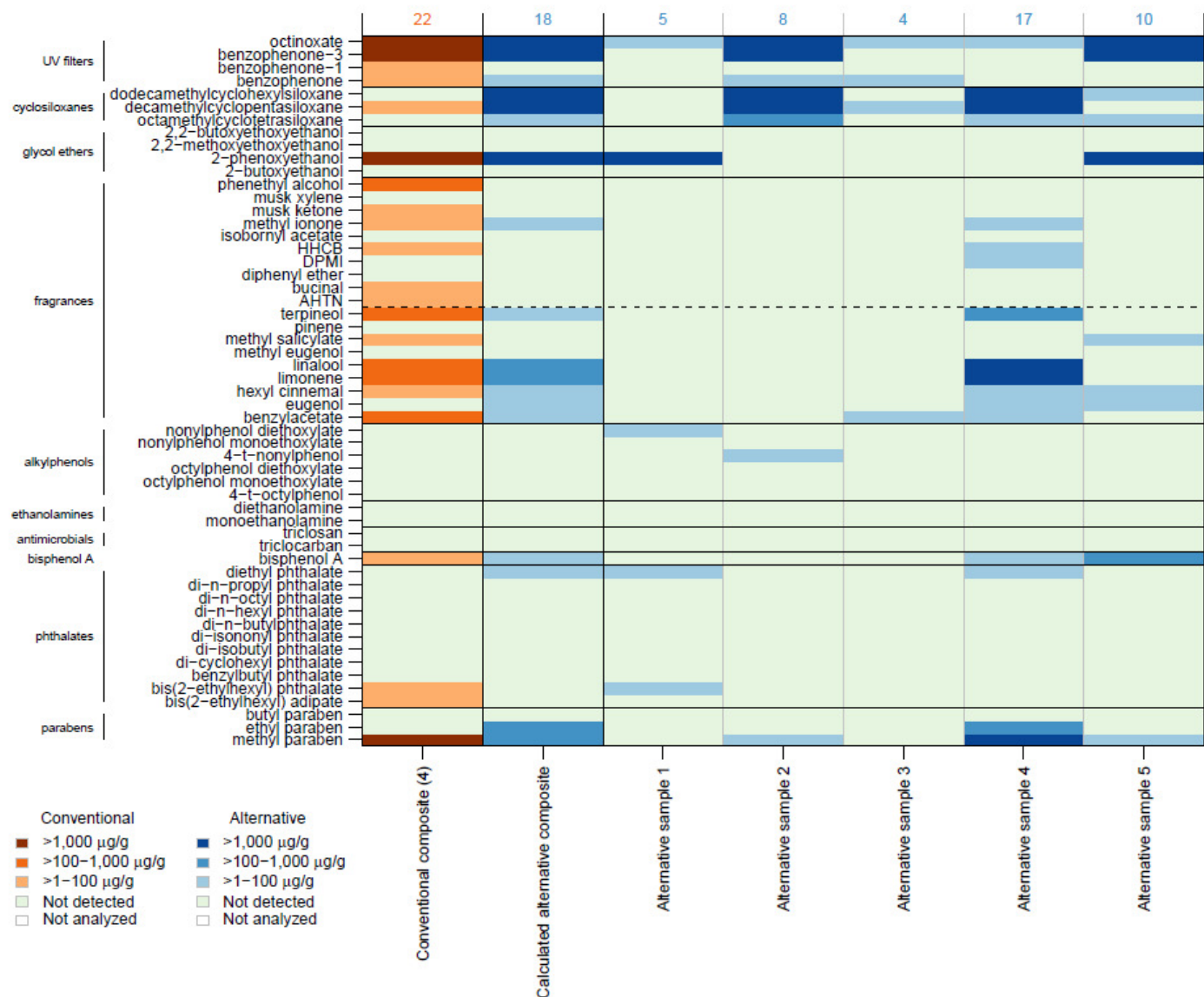


Figure S1. Concentrations of target compounds in sunscreen samples. Compounds are grouped by chemical class, with natural and synthetic fragrances distinguished by a dashed horizontal line. Horizontal (x-axis) shows the conventional sunscreen sample, which was a composite of 4 sunscreens; the calculated composite of 5 alternative sunscreens that were analyzed individually; and then results for each of the 5 alternative sunscreens. Numbers in the top margin count the number of chemicals detected in each sample; numbers in the right margin count number of products containing each compound.

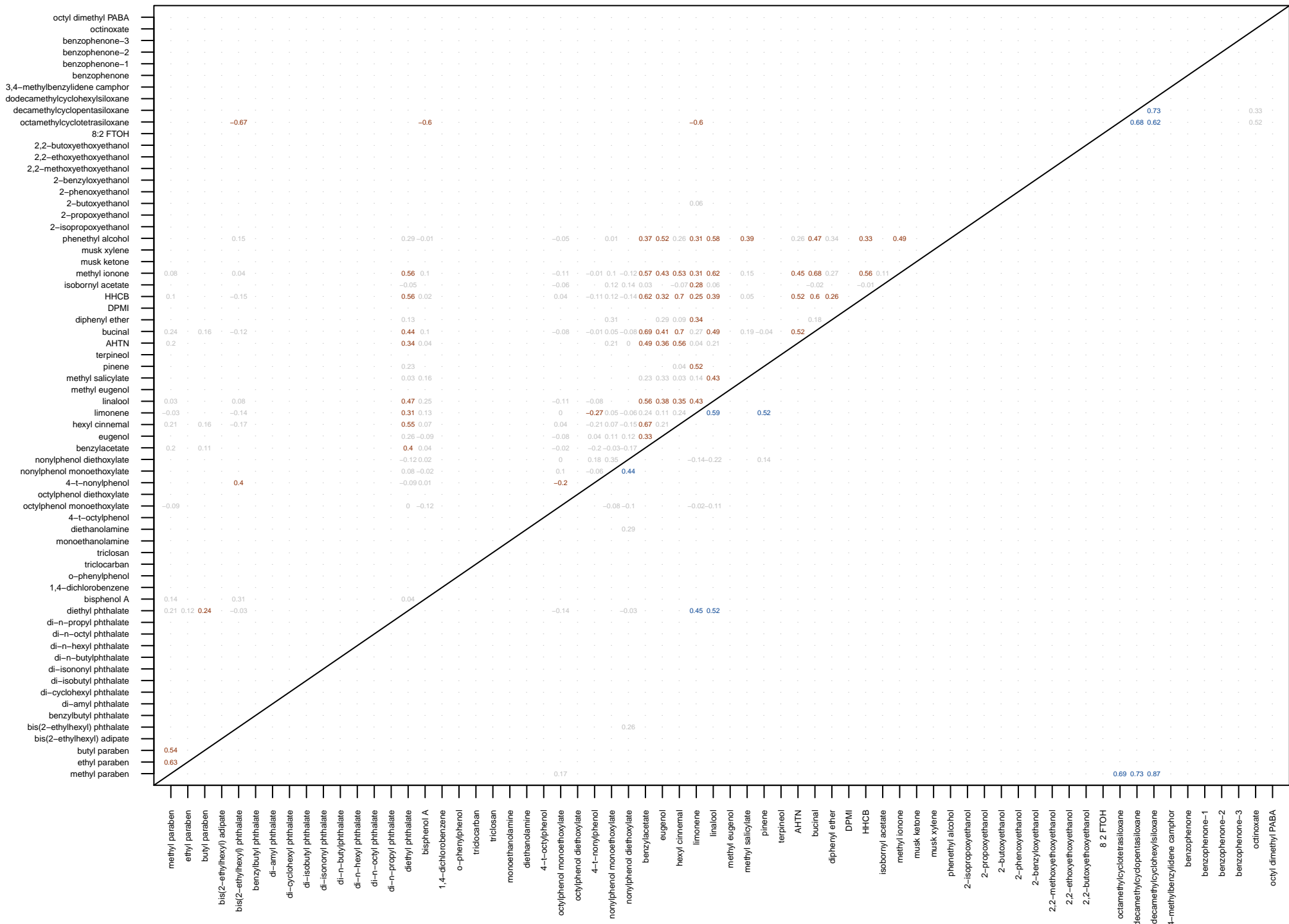


Figure S2. Kendall's tau correlation estimates for concentrations in conventional (upper left; red) and alternative (lower right; blue) products. Significant correlation estimates ( $p < 0.05$ ) in color. '.' indicates insufficient number of detected pairs for correlation analysis. Compounds are sorted by chemical class and match other figures and tables. See the Mixtures section in the manuscript for a discussion of the results.

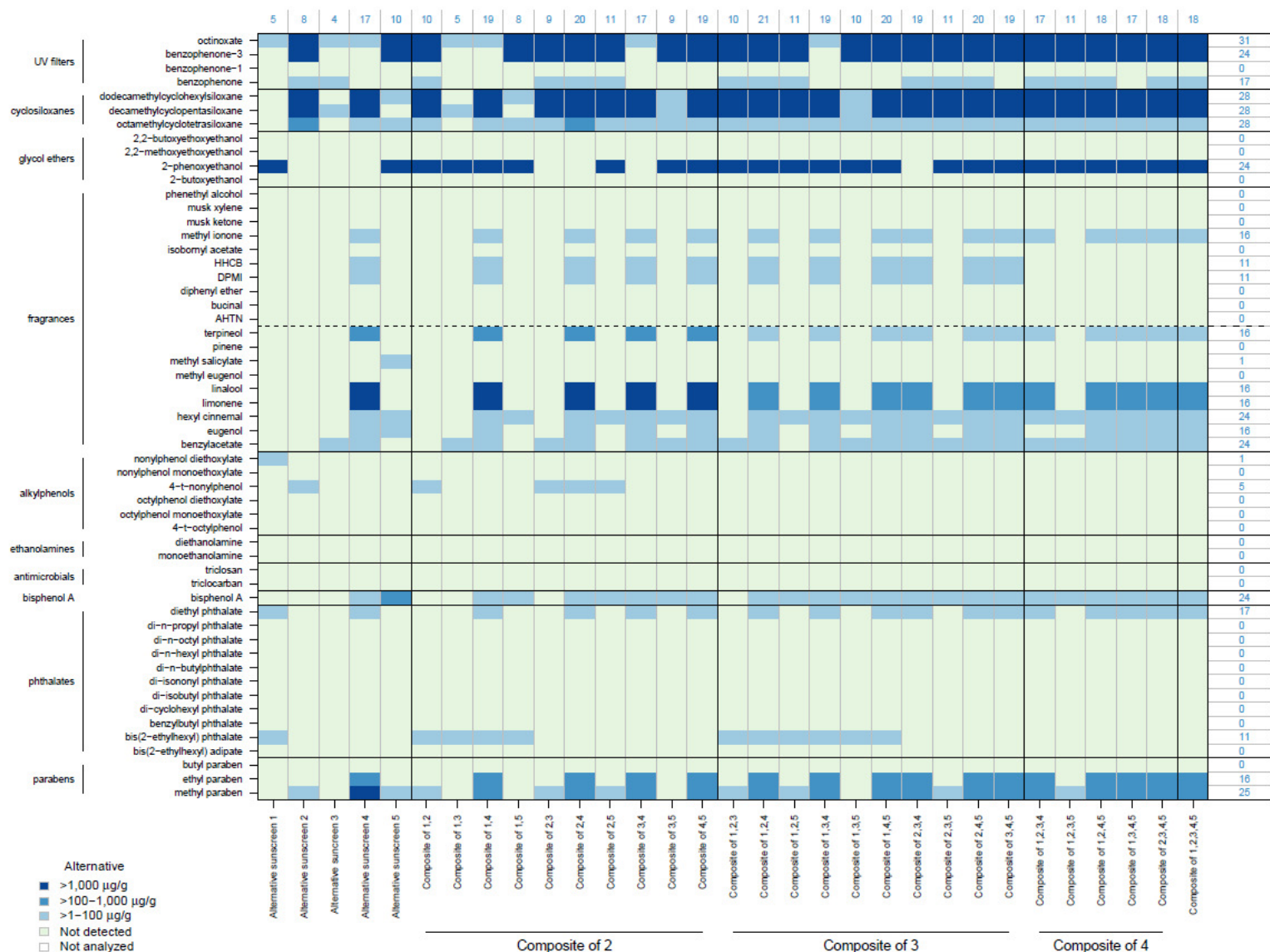


Figure S3. Effects of compositing products on detection patterns: An example using 5 alternative sunscreens. Compounds are grouped by chemical class, with dashed line distinguishing natural and synthetic fragrances. The first 5 samples are the individual sunscreen samples; the remaining are theoretical "composites" using the individual samples. Numbers in the top margin count the number of chemicals detected in composite; numbers in the right margin count number of composites containing each compound.

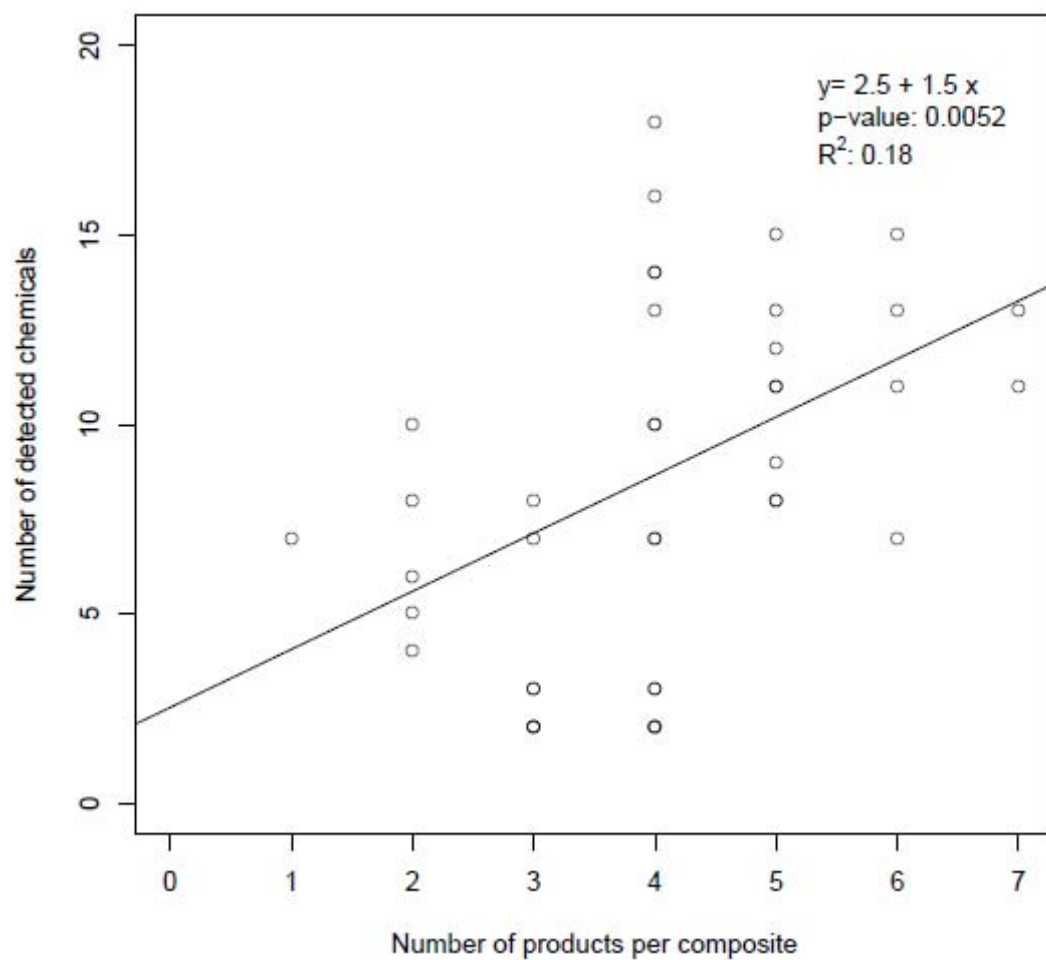


Figure S4. Number of products per composite versus number of detected chemicals for conventional samples. Linear regression model presented in upper right corner with p-value for slope estimate and  $R^2$  value for the model. The number of products per composite and number of chemicals detected have a significant positive relationship.

## **Analytical Quality Assurance/Quality Control (QA/QC) Methods and Results**

To composite samples: for thin liquids, a 1 mL aliquot of each sample was combined and mixed, then 0.25 mL was removed and spiked with the surrogate recovery standards (SRSs), diluted with 50 mL of 3:1 dichloromethane (DCM):methanol, ultra-sonified for 1 min and placed on a shaker table for 15 min; for thick liquids (e.g., toothpaste) and semi-solid materials (e.g., lipstick), approximately 1 g of each product was added in sequence to a tared vial and then mixed with a spatula; 0.25 g was removed, spiked with the SRSs, mixed with 0.5 g muffled Extrelute to form a free-flowing mixture, ultra-sonified and shaken in 50 mL 3:1 DCM:methanol, and filtered as needed through a syringe filter; for solids, equal amounts of each product were finely divided, mixed and 0.25 g was removed, spiked with the SRSs, and extracted as described above. A 6 mL aliquot of each extract was passed through a weak anion exchange SPE cartridge (DSC-NH<sub>2</sub>, 100 mg; Supelco), 1 mL was removed, spiked with the neutral internal standard (IS; bromobiphenyl), and analyzed using GC/MS in the full scan mode for neutral compounds. A separate aliquot of the extract was solvent exchanged into the same volume of methyl-*t*-butyl ether, 1 mL was removed, spiked with the IS dibromophenol-*d*<sub>3</sub> and 50  $\mu$ L pyridine, derivatized with BSTFA with 1% TMCS, and then analyzed using GC/MS in the full scan mode for phenolic compounds. The same phenolic extract was reanalyzed in the multiple ionization detection mode for the multi-component nonylphenol mono- and diethoxylates. The internal standard method of quantification was based on 6 point calibration curves that spanned the range of 0.15-25  $\mu$ g/mL.

QA/QC measures were conducted to ensure accuracy and reliability of measurements. To evaluate potential contamination, we analyzed eight solvent method blanks in round one and five solvent method blanks in round two. To estimate precision we analyzed eight samples in round one and five samples in round 2 as duplicates. Surrogate recoveries were used to characterize accuracy and extraction efficiency.

For each compound, the method reporting limit (MRL) was defined as the maximum of the analytical detection limit and the 90<sup>th</sup> percentile of the blank concentrations within each analytical round. The nominal analytical detection limit was 1  $\mu$ g/g, and so the MRL was above 1  $\mu$ g/g only in cases with detectable concentrations in the blank samples. Concentrations above the MRL were considered quantified and presented in the paper.

Potential sample contamination was evaluated using solvent method blanks (n=13). The target compounds diethyl phthalate, diethanolamine, octylphenol monoethoxylate, octylphenol diethoxylate, nonylphenol monoethoxylate and nonylphenol diethoxylate were detected in at least one blank in the first analytical round and the target compounds methyl paraben, ethyl paraben, butyl paraben, bisphenol A, triclosan, monoethanolamine, diethanolamine, octylphenol diethoxylate, 4-nonylphenol, D4 (octamethylcyclotetrasiloxane), D5 (decamethylcyclopentasiloxane), D6 (dodecamethylcyclohexylsiloxane), benzophenone-1 and benzophenone-3 were detected in at least one blank in the second analytical round. Summary statistics for the solvent blanks for each analytical round are presented in Table S2.

In order to correct potential bias in the reported values, blank correction was performed for chemicals detected in at least 75% of the blanks and were specific to each analytical round. In analytical round one, none of the compounds required blank correction. In analytical round two, one compound (D5; decamethylcyclopentasiloxane) was blank corrected by subtracting the median blank concentration from the reported values, resulting in a median 87% change and maximum 200% change to reported concentration.

Precision is presented as the relative percent difference between duplicate pair concentrations (Table S3). Summary statistics were calculated only using pairs of detected values. In general, for the 28 analytes with pairs of detected values, precision estimates were <50%, except in 2 instances (ethyl paraben and 4-nonylphenol). There were 7 analytes with “mismatched” pairs, meaning that one of the duplicate pairs was detected and one was not.

Five surrogate compounds (octyl alcohol-d17, 4-chlorophenyl phenyl ether-d5, di-n-butyl phthalate-d4, phenanthrene-d10 and bisphenol A-d16) were spiked into samples prior to extraction at 1 µg/ml level (or 200 µg/g; levels of octyl alcohol-d17 increased to 2 µg/ml in the second analytical round for increased sensitivity) to evaluate accuracy and extraction efficiency. Median percent recoveries were within the 50-150% acceptance range for all surrogates over both analytical rounds (Figure S5). There were sporadic recoveries outside of this range in the 71 Round 1 samples for bisphenol A-d16 (below 50% in 5 samples and above 150% in 6 samples), and octyl alcohol-d17 (below 50% in 23 samples and above 150% in 1 sample). Variable recoveries may be attributable to interferences from complex matrices. Reported concentrations were not adjusted or corrected.

Six products were spiked prior to extraction with the full suite of analytes at concentrations of 100 ng/ml for the alkylphenol ethoxylates and 2.5 µg/ml for all other compounds, and analyzed to assess recovery. Three types of conventional and alternative products were selected to represent different matrices: glass cleaner (liquid), sunscreen (cream), and scrubbing powder (semi-solid). Thirteen recovery estimates (of 406 possible) could not be estimated due to matrix interference. Median recoveries across all products were within 50-150%, except for benzophenone-2 (not detected in any samples), monoethanolamine, and diethanolamine, which had low recoveries (Table S4). Therefore, the results presented for these compounds may be underestimates of the true concentrations. There were no significant differences in recoveries across product type ( $p>0.05$ ).

Table S2. Summary statistics for solvent method blanks (µg/g equivalent<sup>a</sup>) in each analytical round.

| Compound                    | Chemical Class | Round 1       |                |      |        |      |     | Round 2       |                |      |        |      |     |
|-----------------------------|----------------|---------------|----------------|------|--------|------|-----|---------------|----------------|------|--------|------|-----|
|                             |                | No. of Blanks | No. of Detects | Min. | Median | Max. | MRL | No. of Blanks | No. of Detects | Min. | Median | Max. | MRL |
| methyl paraben              | parabens       | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 2    | 1.2 |
| ethyl paraben               | parabens       | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 2    | 1.2 |
| butyl paraben               | parabens       | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 4    | 2.4 |
| bis(2-ethylhexyl) adipate   | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| bis(2-ethylhexyl) phthalate | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| benzylbutyl phthalate       | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-amyl phthalate           | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-cyclohexyl phthalate     | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-isobutyl phthalate       | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-isononyl phthalate       | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-n-butylphthalate         | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-n-hexyl phthalate        | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-n-octyl phthalate        | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| di-n-propyl phthalate       | phthalates     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| diethyl phthalate           | phthalates     | 8             | 2              | 0    | 0      | 4    | 2.6 | 5             | 0              | 0    | 0      | 0    | 1   |
| bisphenol A                 | bisphenol A    | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 4    | 2.4 |
| 1,4-dichlorobenzene         | antimicrobials | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| o-phenylphenol              | antimicrobials | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| triclocarban                | antimicrobials | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| triclosan                   | antimicrobials | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 4    | 2.4 |
| monoethanolamine            | ethanolamines  | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 4    | 2.4 |
| diethanolamine              | ethanolamines  | 8             | 1              | 0    | 0      | 2    | 1   | 5             | 1              | 0    | 0      | 2    | 1.2 |
| 4-t-octylphenol             | alkylphenols   | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| octylphenol monoethoxylate  | alkylphenols   | 8             | 4              | 0    | 0.022  | 0.15 | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| octylphenol diethoxylate    | alkylphenols   | 8             | 5              | 0    | 0.04   | 0.35 | 1   | 5             | 1              | 0    | 0      | 1    | 1   |
| 4-t-nonylphenol             | alkylphenols   | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 1              | 0    | 0      | 0.4  | 1   |
| nonylphenol monoethoxylate  | alkylphenols   | 8             | 2              | 0    | 0      | 0.35 | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| nonylphenol diethoxylate    | alkylphenols   | 8             | 3              | 0    | 0      | 0.71 | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| benzylacetate               | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| eugenol                     | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| hexyl cinnemal              | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| limonene                    | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| linalool                    | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| methyl eugenol              | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| methyl salicylate           | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |

| Compound                                  | Chemical Class | Round 1       |                |      |        |      |     | Round 2       |                |      |        |      |     |
|---|----------------|---------------|----------------|------|--------|------|-----|---------------|----------------|------|--------|------|-----|
|   |                | No. of Blanks | No. of Detects | Min. | Median | Max. | MRL | No. of Blanks | No. of Detects | Min. | Median | Max. | MRL |
| pinene                                    | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| terpineol                                 | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| AHTN                                      | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| bucinal                                   | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| diphenyl ether                            | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| DPMI                                      | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| HHCB                                      | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| isobornyl acetate                         | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| methyl ionone                             | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| musk ketone                               | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| musk xylene                               | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| phenethyl alcohol                         | fragrances     | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| 2-isopropoxyethanol                       | glycol ethers  | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| 2-propoxyethanol                          | glycol ethers  | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| 2-butoxyethanol                           | glycol ethers  | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| 2-phenoxyethanol                          | glycol ethers  | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| 2-benzyloxyethanol                        | glycol ethers  | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| 2,2-methoxyethoxyethanol                  | glycol ethers  | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| 2,2-ethoxyethoxyethanol                   | glycol ethers  | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| 2,2-butoxyethoxyethanol                   | glycol ethers  | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| 8:2 FTOH                                  | perfluorinated | 8             | 0              | 0    | 0      | 0    | 1   | 5             | 0              | 0    | 0      | 0    | 1   |
| octamethylcyclotetrasiloxane              | cyclosiloxanes | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 3              | 0    | 2      | 6    | 5.2 |
| decamethylcyclopentasiloxane <sup>b</sup> | cyclosiloxanes | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 5              | 2    | 6      | 32   | 17  |
| dodecamethylcyclohexylsiloxane            | cyclosiloxanes | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 2              | 0    | 0      | 2    | 2   |
| 3,4-methylbenzylidene camphor             | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| benzophenone                              | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| benzophenone-1                            | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 1              | 0    | 0      | 2    | 1.2 |
| benzophenone-2                            | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| benzophenone-3                            | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 1              | 0    | 0      | 8    | 4.8 |
| octinoxate                                | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |
| octyl dimethyl PABA                       | UV filters     | NA            | NA             | NA   | NA     | NA   | NA  | 5             | 0              | 0    | 0      | 0    | 1   |

NA indicates "not applicable" since compound was added during second analytical round

MRL represents the method reporting limit, which is the maximum of the 90th percentile of the blanks or the analytical detection limit (1 ug/g). MRLs have been blank corrected when necessary.

<sup>a</sup> Calculated assuming 50 ml extract volume and 0.25 g sample, which was used for all product samples

<sup>b</sup> Subjected to blank correction by subtracting median blank concentration from reported values

Table S3. Summary statistics for precision, calculated as relative percent difference (%).

| Compound                    | Chemical Class | No. of Duplicate Pairs | No. of Detected Pairs | No. of Mismatched Pairs <sup>a</sup> | No. of Nondetect Pairs | Median <sup>b</sup> | Max. <sup>b</sup> |
|-----------------------------|----------------|------------------------|-----------------------|--------------------------------------|------------------------|---------------------|-------------------|
| methyl paraben              | parabens       | 9                      | 3                     | 0                                    | 6                      | 22                  | 38                |
| ethyl paraben               | parabens       | 9                      | 1                     | 0                                    | 8                      | 67                  | 67                |
| butyl paraben               | parabens       | 9                      | 2                     | 0                                    | 7                      | 36                  | 54                |
| bis(2-ethylhexyl) adipate   | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| bis(2-ethylhexyl) phthalate | phthalates     | 9                      | 3                     | 1                                    | 5                      | 46                  | 67                |
| benzylbutyl phthalate       | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| di-amyl phthalate           | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| di-cyclohexyl phthalate     | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| di-isobutyl phthalate       | phthalates     | 9                      | 0                     | 1                                    | 8                      | ND                  | ND                |
| di-isononyl phthalate       | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| di-n-butylphthalate         | phthalates     | 9                      | 0                     | 1                                    | 8                      | ND                  | ND                |
| di-n-hexyl phthalate        | phthalates     | 9                      | 0                     | 1                                    | 8                      | ND                  | ND                |
| di-n-octyl phthalate        | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| di-n-propyl phthalate       | phthalates     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| diethyl phthalate           | phthalates     | 9                      | 3                     | 1                                    | 5                      | 0.84                | 6.9               |
| bisphenol A                 | bisphenol A    | 9                      | 1                     | 0                                    | 8                      | 0                   | 0                 |
| 1,4-dichlorobenzene         | antimicrobials | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| o-phenylphenol              | antimicrobials | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| triclocarban                | antimicrobials | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| triclosan                   | antimicrobials | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| monoethanolamine            | ethanolamines  | 9                      | 1                     | 0                                    | 8                      | 36                  | 36                |
| diethanolamine              | ethanolamines  | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| 4-t-octylphenol             | alkylphenols   | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| octylphenol monoethoxylate  | alkylphenols   | 9                      | 5                     | 0                                    | 4                      | 21                  | 67                |
| octylphenol diethoxylate    | alkylphenols   | 9                      | 7                     | 0                                    | 2                      | 45                  | 75                |
| 4-t-nonylphenol             | alkylphenols   | 9                      | 2                     | 0                                    | 7                      | 64                  | 100               |
| nonylphenol monoethoxylate  | alkylphenols   | 9                      | 1                     | 3                                    | 4                      | 7.5                 | 7.5               |
| nonylphenol diethoxylate    | alkylphenols   | 9                      | 4                     | 2                                    | 3                      | 50                  | 83                |
| benzylacetate               | fragrances     | 9                      | 2                     | 0                                    | 7                      | 12                  | 18                |
| eugenol                     | fragrances     | 9                      | 2                     | 0                                    | 7                      | 5.2                 | 10                |
| hexyl cinnemal              | fragrances     | 9                      | 2                     | 0                                    | 7                      | 7.8                 | 9.8               |
| limonene                    | fragrances     | 9                      | 3                     | 0                                    | 6                      | 0                   | 7.2               |
| linalool                    | fragrances     | 9                      | 2                     | 0                                    | 7                      | 11                  | 12                |
| methyl eugenol              | fragrances     | 9                      | 1                     | 0                                    | 8                      | 0                   | 0                 |
| methyl salicylate           | fragrances     | 9                      | 1                     | 0                                    | 8                      | 0                   | 0                 |
| pinene                      | fragrances     | 9                      | 1                     | 0                                    | 8                      | 8.7                 | 8.7               |
| terpineol                   | fragrances     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |

| Compound                       | Chemical Class | No. of Duplicate Pairs | No. of Detected Pairs | No. of Mismatched Pairs <sup>a</sup> | No. of Nondetect Pairs | Median <sup>b</sup> | Max. <sup>b</sup> |
|--------------------------------|----------------|------------------------|-----------------------|--------------------------------------|------------------------|---------------------|-------------------|
| AHTN                           | fragrances     | 9                      | 2                     | 0                                    | 7                      | 16                  | 18                |
| bucinal                        | fragrances     | 9                      | 2                     | 0                                    | 7                      | 9.7                 | 11                |
| diphenyl ether                 | fragrances     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| DPMI                           | fragrances     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| HHCB                           | fragrances     | 9                      | 2                     | 0                                    | 7                      | 12                  | 21                |
| isobornyl acetate              | fragrances     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| methyl ionone                  | fragrances     | 9                      | 2                     | 0                                    | 7                      | 12                  | 15                |
| musk ketone                    | fragrances     | 9                      | 1                     | 0                                    | 8                      | 3.5                 | 3.5               |
| musk xylene                    | fragrances     | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| phenethyl alcohol              | fragrances     | 9                      | 1                     | 0                                    | 8                      | 13                  | 13                |
| 2-isopropoxyethanol            | glycol ethers  | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| 2-propoxyethanol               | glycol ethers  | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| 2-butoxyethanol                | glycol ethers  | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| 2-phenoxyethanol               | glycol ethers  | 1                      | 1                     | 0                                    | 0                      | 6.6                 | 6.6               |
| 2-benzyloxyethanol             | glycol ethers  | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| 2,2-methoxyethoxyethanol       | glycol ethers  | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| 2,2-ethoxyethoxyethanol        | glycol ethers  | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| 2,2-butoxyethoxyethanol        | glycol ethers  | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| 8:2 FTOH                       | perfluorinated | 9                      | 0                     | 0                                    | 9                      | ND                  | ND                |
| octamethylcyclotetrasiloxane   | cyclosiloxanes | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| decamethylcyclopentasiloxane   | cyclosiloxanes | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| dodecamethylcyclohexylsiloxane | cyclosiloxanes | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| 3,4-methylbenzylidene camphor  | UV filters     | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| benzophenone                   | UV filters     | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| benzophenone-1                 | UV filters     | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| benzophenone-2                 | UV filters     | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| benzophenone-3                 | UV filters     | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |
| octinoxate                     | UV filters     | 1                      | 1                     | 0                                    | 0                      | 0                   | 0                 |
| octyl dimethyl PABA            | UV filters     | 1                      | 0                     | 0                                    | 1                      | ND                  | ND                |

ND indicates insufficient number of detected pairs to calculate precision

<sup>a</sup> Mismatched pairs are those pairs where one sample is detected and the other is not

<sup>b</sup> Summary statistics calculated using duplicate pairs where both samples are detected

Table S4. Summary statistics for recoveries (%) from spiked products

| Compound                    | Chemical Class | No. of Spiked Samples | Min. | Median | Mean | Max. |
|-----------------------------|----------------|-----------------------|------|--------|------|------|
| methyl paraben              | parabens       | 5                     | 65   | 78     | 76   | 83   |
| ethyl paraben               | parabens       | 6                     | 73   | 76     | 77   | 82   |
| butyl paraben               | parabens       | 6                     | 77   | 78     | 79   | 84   |
| bis(2-ethylhexyl) adipate   | phthalates     | 6                     | 96   | 114    | 112  | 126  |
| bis(2-ethylhexyl) phthalate | phthalates     | 6                     | 105  | 115    | 115  | 123  |
| benzylbutyl phthalate       | phthalates     | 6                     | 92   | 109    | 111  | 125  |
| di-amyl phthalate           | phthalates     | 6                     | 108  | 113    | 115  | 124  |
| di-cyclohexyl phthalate     | phthalates     | 6                     | 105  | 116    | 116  | 125  |
| di-isobutyl phthalate       | phthalates     | 6                     | 112  | 118    | 119  | 128  |
| di-isononyl phthalate       | phthalates     | 6                     | 98   | 114    | 112  | 120  |
| di-n-butyl phthalate        | phthalates     | 6                     | 112  | 116    | 118  | 126  |
| di-n-hexyl phthalate        | phthalates     | 6                     | 102  | 112    | 114  | 126  |
| di-n-octyl phthalate        | phthalates     | 6                     | 82   | 112    | 109  | 122  |
| d-n-propyl phthalate        | phthalates     | 6                     | 112  | 116    | 117  | 124  |
| diethyl phthalate           | phthalates     | 6                     | 110  | 116    | 116  | 122  |
| bisphenol A                 | bisphenol A    | 6                     | 74   | 80     | 81   | 88   |
| 1,4-dichlorobenzene         | antimicrobials | 6                     | 59   | 94     | 90   | 113  |
| o-phenylphenol              | antimicrobials | 6                     | 78   | 84     | 84   | 92   |
| triclocarban                | antimicrobials | 6                     | 49.5 | 72     | 71.5 | 91.5 |
| triclosan                   | antimicrobials | 6                     | 72   | 76     | 77   | 84   |
| monoethanolamine            | ethanolamines  | 5                     | 0    | 9      | 14   | 44   |
| diethanolamine              | ethanolamines  | 6                     | 0    | 22     | 33   | 99   |
| 4-t-octylphenol             | alkylphenols   | 6                     | 81   | 84     | 86   | 93   |
| octylphenol monoethoxylate  | alkylphenols   | 6                     | 82   | 84     | 88   | 110  |
| octylphenol diethoxylate    | alkylphenols   | 6                     | 55   | 62     | 64   | 76   |
| 4-t-nonylphenol             | alkylphenols   | 5                     | 50   | 67     | 65   | 78   |
| nonylphenol monoethoxylate  | alkylphenols   | 4                     | 85   | 90     | 92   | 103  |
| nonylphenol diethoxylate    | alkylphenols   | 6                     | 59   | 76     | 117  | 355  |
| benzyl acetate              | fragrances     | 6                     | 92   | 100    | 101  | 110  |
| eugenol                     | fragrances     | 6                     | 67   | 73     | 73   | 78   |
| hexyl cinnemal              | fragrances     | 6                     | 100  | 110    | 110  | 119  |
| limonene                    | fragrances     | 6                     | 60   | 90     | 90   | 118  |
| linalool                    | fragrances     | 6                     | 86   | 110    | 109  | 121  |
| methyl eugenol              | fragrances     | 6                     | 101  | 108    | 108  | 114  |
| methyl salicylate           | fragrances     | 6                     | 23   | 66     | 59   | 73   |
| pinene                      | fragrances     | 6                     | 46   | 80     | 81   | 118  |
| terpineol                   | fragrances     | 6                     | 53   | 96     | 92   | 113  |
| diphenyl ether              | fragrances     | 6                     | 113  | 118    | 119  | 126  |
| isobornyl acetate           | fragrances     | 6                     | 104  | 121    | 118  | 123  |
| phenethyl alcohol           | fragrances     | 6                     | 62   | 92     | 89   | 102  |
| AHTN                        | fragrances     | 6                     | 118  | 123    | 124  | 131  |
| bucinal                     | fragrances     | 6                     | 28   | 70     | 61   | 80   |
| DPMI                        | fragrances     | 6                     | 111  | 122    | 120  | 124  |
| HHCB                        | fragrances     | 6                     | 113  | 118    | 118  | 122  |
| methyl ionone               | fragrances     | 6                     | 114  | 123    | 121  | 125  |
| musk ketone                 | fragrances     | 6                     | 96   | 108    | 107  | 116  |
| musk xylene                 | fragrances     | 6                     | 87   | 115    | 113  | 132  |
| 2-isopropoxyethanol         | glycol ethers  | 6                     | 49   | 70     | 74   | 104  |
| 2-propoxyethanol            | glycol ethers  | 6                     | 34   | 59     | 58   | 74   |

| Compound                       | Chemical Class | No. of Spiked Samples | Min. | Median | Mean | Max. |
|--------------------------------|----------------|-----------------------|------|--------|------|------|
| 2-butoxyethanol                | glycol ethers  | 5                     | 52   | 91     | 88   | 114  |
| 2-phenoxyethanol               | glycol ethers  | 5                     | 78   | 82     | 86   | 99   |
| 2-benzyloxyethanol             | glycol ethers  | 6                     | 5    | 78     | 67   | 83   |
| 2,2-methoxyethoxyethanol       | glycol ethers  | 6                     | 46   | 101    | 92   | 117  |
| 2,2-ethoxyethoxyethanol        | glycol ethers  | 6                     | 97   | 105    | 104  | 107  |
| 2,2-butoxyethoxyethanol        | glycol ethers  | 6                     | 50   | 84     | 77   | 96   |
| 8:2 FTOH                       | perfluorinated | 6                     | 94   | 116    | 115  | 143  |
| octamethylcyclotetrasiloxane   | cyclosiloxanes | 6                     | 51   | 90     | 91   | 133  |
| decamethylcyclopentasiloxane   | cyclosiloxanes | 5                     | 81   | 105    | 108  | 135  |
| dodecamethylcyclohexylsiloxane | cyclosiloxanes | 5                     | 105  | 119    | 118  | 130  |
| 3,4-methylbenzylidene camphor  | UV filters     | 6                     | 116  | 119    | 120  | 126  |
| benzophenone                   | UV filters     | 6                     | 104  | 116    | 115  | 122  |
| benzophenone-1                 | UV filters     | 6                     | 37   | 70     | 64   | 80   |
| benzophenone-2                 | UV filters     | 6                     | 0    | 18     | 17   | 34   |
| benzophenone-3                 | UV filters     | 4                     | 33   | 64     | 58   | 70   |
| octinoxate                     | UV filters     | 4                     | 130  | 161    | 154  | 165  |
| octadimethyl PABA              | UV filters     | 6                     | 92   | 112    | 110  | 118  |

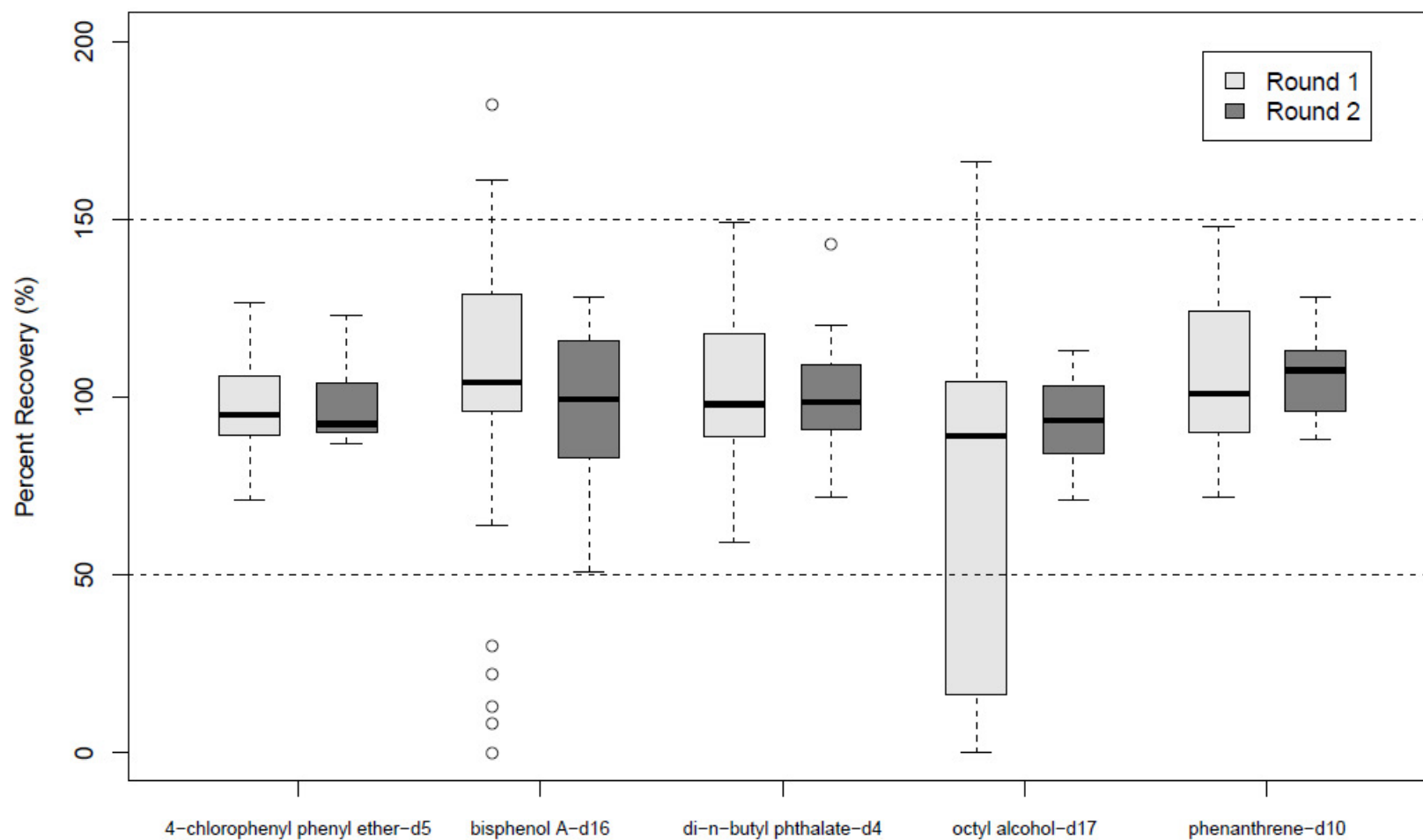


Figure S5. Surrogate recovery distributions for five surrogates for each analytical round. For each surrogate standard, there are 71 samples from Round 1 and 14 samples from Round 2. Surrogates were spiked at 1  $\mu\text{g/ml}$  (200  $\mu\text{g/g}$ ), except for octyl alcohol-d17 in Round 2, which as increased to 2  $\mu\text{g/ml}$  (400  $\mu\text{g/g}$ ) to increase sensitivity.

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